

# PARAMETERIZATIONS AND FITTING OF BI-DIRECTED GRAPH MODELS TO CATEGORICAL DATA

MONIA LUPPARELLI

*Dipartimento di Economia Politica e Metodi Quantitativi,  
via S. Felice, 7, 27100, Pavia, Italy*

GIOVANNI M. MARCHETTI

*Dipartimento di Statistica “G. Parenti”,  
viale Morgagni, 59, 50134, Florence, Italy*

WICHER P. BERGSMA

*London School of Economics and Political Science,  
Houghton Street, WC2A 2AE London, UK*

**ABSTRACT.** We discuss two parameterizations of models for marginal independencies for discrete distributions which are representable by bi-directed graph models, under the global Markov property. Such models are useful data analytic tools especially if used in combination with other graphical models. The first parameterization, in the saturated case, is also known as the multivariate logistic transformation, the second is a variant that allows, in some (but not all) cases, variation independent parameters. An algorithm for maximum likelihood fitting is proposed, based on an extension of the Aitchison and Silvey method.

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*E-mail addresses:* `mlupparelli@eco.unipv.it`, `giovanni.marchetti@ds.unifi.it`,  
`W.P.Bergsma@lse.ac.uk`.

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## 1. INTRODUCTION

This paper deals with the parametrization and fitting of a class of marginal independence models for multivariate discrete distributions. These models are associated to a class of graphs where the missing edges represent marginal independence. The graphs used have special edges to distinguish them from undirected graphs used to encode conditional independencies. Cox & Wermuth (1993) use dashed edges and call the graphs covariance graphs by stressing the equivalence between a marginal pairwise independence and a zero covariance in a Gaussian distribution. Richardson & Spirtes (2002) use instead bi-directed edges following the tradition of path analysts. The interpretation of the graphs in terms of independencies is based on the pairwise and global Markov properties discussed originally by Kauermann (1996) for covariance graphs and later developed by Richardson (2003). These are recalled in Section 2.

Models of marginal independence can be useful in several contexts. For instance, Cox & Wermuth (1993) present an example on diabetic patients concerning four continuous variables:  $X_1$ , the duration of the illness,  $X_2$ , the quantity of a particular metabolic parameter,  $X_3$ , a score for the knowledge about the illness, and  $X_4$ , a questionnaire score measuring a patients' attitude called external fatalism. The structure of the correlation matrix suggests for this data set the marginal independencies  $X_4 \perp\!\!\!\perp \{X_1, X_2\}$  and  $X_1 \perp\!\!\!\perp \{X_3, X_4\}$ . This marginal independence model can be represented by the bi-directed graph in Figure 1(a), called a 4-chain. The suggested interpretation is that the duration of illness  $X_1$  and the external fatalism  $X_4$  are independent explanatory variables of the responses  $X_2, X_3$  in two seemingly unrelated regressions. For further discussion on the interpretation of covariance chains see (Wermuth *et al.*, 2006). Bi-directed graph models are sometimes useful to represent marginal independence structures induced after marginalizing over latent variables. The independence structure of the diabetes data, for example, might be represented by assuming an underlying generating process described by a directed acyclic graph, shown in Figure 1(b), with one latent variable pointing both to  $X_2$  and  $X_3$ . After marginalizing over the latent variable the induced independencies are exactly those encoded in the bi-directed graph of Figure 1(a). As another example with four binary variables, consider the data by Coppen (1966) shown in Table 1, concerning symptoms of 362 psychiatric patients. The symptoms are:  $X_1$  : stability,  $X_2$  : validity,

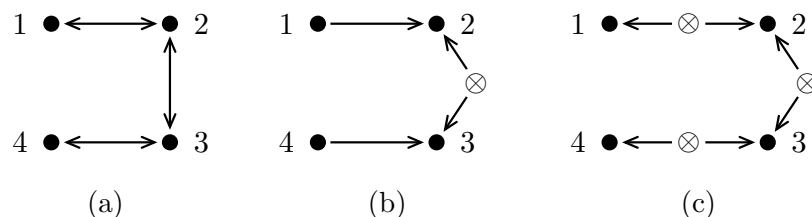


FIGURE 1. (a) A bi-directed graph, called 4-chain, implying the independencies:  $4 \perp\!\!\!\perp 12$  and  $1 \perp\!\!\!\perp 34$ . Directed acyclic graphs inducing the same independencies after marginalization over the latent variables (with nodes  $\otimes$ ): (b) with one latent variable; (c) with 3 latent variables.

$X_3$  : acute depression and  $X_4$  : solidity. The chi-squared tests of the hypotheses of marginal independence  $X_4 \perp\!\!\!\perp \{X_1, X_2\}$  and  $X_1 \perp\!\!\!\perp \{X_3, X_4\}$ , with p-values, respectively, 0.32 and 0.14, are separately not significant and the independence model defined by the two statements jointly gives a satisfactory fit with a deviance of 8.61 on 5 degrees of freedom. Thus the same bi-directed graph model defined by the 4-chain of Figure 1(a) is adequate. In Section 6 we discuss the details of this application. In this example, if all symptoms are treated on the same footing, it is less plausible that a single latent variable will explain the independence structure and more (at least three) latent variables are required to suggest a generating process, as shown in the graph of Figure 1(c).

Developing a parameterization for Gaussian bi-directed graph models is straightforward since the pairwise and the global Markov property are equivalent and they can be simply fulfilled by constraining to zero a subset of covariances. Accomplishing the same task in the discrete case is much more difficult due to the high number of parameters and to the non-equivalence of the two Markov properties. Recently, Drton & Richardson (2007) studied the parametrization of bi-directed graph models for discrete binary distributions, based on Möbius parameters, by proposing a version of their iterative conditional fitting algorithm for maximum likelihood estimation.

In this paper we propose different parameterizations, suitable for general categorical variables, based on the class of marginal log-linear models of Bergsma & Rudas (2002). One special case of this class, especially useful in the context of bi-directed graph models, is the multivariate logistic parameterization of Glonek & McCullagh (1995); see also Kauermann (1997). We discuss a further marginal log-linear parametrization that can, in special cases, be shown to imply variation independent parameters. We show that the marginal log-linear parameterizations suggest a class of reduced models defined by constraining certain higher-order log-linear parameters to zero. Then we discuss maximum likelihood estimation of the models and we propose a general algorithm based on previous works by Aitchison & Silvey (1958), Lang (1996), Bergsma (1997).

The remainder of this paper is organized as follows. Section 2 reviews discrete bi-directed graphs and their Markov properties. In Section 3 we give the essential results concerning the theory of marginal log-linear models. Two parameterizations of bi-directed graph models are given then in Section 4 illustrating their properties with special emphasis on variation independence and the interpretation of the parameters. In Section 5 we

TABLE 1. *Data by Coppen (1966) on symptoms of psychiatric patients. The variables are  $X_1$  : stability (1=extroverted, 2=introverted),  $X_2$  : validity (1=psychasthenic, 2=energetic),  $X_3$  : depression (yes, no),  $X_4$  : solidity (1=hysterical, 2=rigid).*

$X_1$	$X_3$	$X_4$		1		2	
		$X_2$		1	2	1	2
1	y			15	30	9	32
	n			25	22	46	27
2	y			23	22	14	16
	n			14	8	47	12

propose an algorithm for maximum likelihood fitting and then, in Section 6 we provide some examples. Finally, in Section 7 we give a short discussion, with a comparison with the approach by Drton & Richardson (2007).

## 2. DISCRETE BI-DIRECTED GRAPH MODELS

Bi-directed graphs are essentially undirected graphs with edges represented by bi-directed arrows instead of full lines. We review in this section the main concepts of graph theory required to understand the models. A bi-directed graph  $G = (V, E)$  is a pair  $G = (V, E)$ , where  $V = \{1, \dots, d\}$  is a set of nodes, and  $E$  is a set of edges defined by two-element subsets of  $V$ . Two nodes  $u, v$  are *adjacent* or neighbours if  $uv$  is an edge of  $G$  and in this case the edge is drawn as bi-directed,  $u \longleftrightarrow v$ . Two edges are adjacent if they have an end node in common. A *path* from a node  $u$  to a node  $v$  is a sequence of adjacent edges connecting  $u$  and  $v$  for which the corresponding sequence of nodes contains no repetitions. The nodes  $u$  and  $v$  are called the *endpoints* of the path and all the other nodes are called the *inner nodes*.

A graph  $G$  is *complete* if all its nodes are pairwise adjacent. A non-empty graph  $G$  is called *connected* if any two of its nodes are linked by a path in  $G$ , otherwise it is called *disconnected*. If  $A$  is a subset of the node set  $V$  of  $G$ , the graph  $G_A$  with nodes  $A$  and containing all the edges of  $G$  with endpoints in  $A$  is called an *induced subgraph*. If a subgraph  $G_A$  is connected (resp. disconnected, complete) we call also  $A$  connected (resp. disconnected, complete), in  $G$ . The set of all disconnected sets of the graph  $G$  will be denoted by  $\mathcal{D}$ , and the set of all the connected sets of  $G$  will be denoted by  $\mathcal{C}$ . In a graph  $G$  a *connected component* or simply a component is a maximal connected subgraph. If a subset  $D$  of nodes is disconnected then it can be uniquely decomposed into more connected components  $C_1, \dots, C_r$ , say, such that  $D = C_1 \cup \dots \cup C_r$ .

The usual notion of separation in undirected graphs can be used also for bi-directed graphs. Thus, given three disjoint subsets of nodes  $A$ ,  $B$  and  $C$ ,  $A$  and  $B$  are said to be *separated by  $C$*  if for any  $u$  in  $A$  and any  $v$  in  $B$  all paths from  $u$  to  $v$  have at least one inner node in  $C$ . The cardinality of a set  $V$  will be denoted by  $|V|$ . The set of all the subsets of  $V$ , the power set, will be denoted by  $\mathcal{P}(V)$ . We use also the notation  $\mathcal{P}_0(V)$  for the set of all nonempty subsets of  $V$ .

Let  $X = (X_v, v \in V)$  be a discrete random vector with each component  $X_v$  taking on values in the finite set  $\mathcal{I}_v = \{1, \dots, b_v\}$ . The Cartesian product  $\mathcal{I}_V = \times_{v \in V} \mathcal{I}_v$ , is a contingency table, with generic element  $\mathbf{i} = (i_v, v \in V)$ , called a cell of the table, and with total number of cells  $t = |\mathcal{I}_V|$ . We assume that  $X$  has a joint probability function  $p(\mathbf{i})$ ,  $\mathbf{i} \in \mathcal{I}_V$  giving the probability that an individual falls in cell  $\mathbf{i}$ . Given a subset  $M \subseteq V$  of the variables, the marginal contingency table is  $\mathcal{I}_M = \times_{v \in M} \mathcal{I}_v$  with generic cell  $\mathbf{i}_M$  and the marginal probability function of the random vector  $X_M = (X_v, v \in M)$  is  $p_M(\mathbf{i}_M) = \sum_{\mathbf{j} \in \mathcal{I}_V | \mathbf{j}_M = \mathbf{i}_M} p(\mathbf{j})$ .

A bi-directed graph  $G = (V, E)$  induces an independence model for the discrete random vector  $X = (X_v, v \in V)$  by defining a Markov property, i.e. a rule for reading off the graph the independence relations. In the following we shall use the shorthand notation  $A \perp\!\!\!\perp B | C$  to indicate the conditional independence  $X_A \perp\!\!\!\perp X_B | X_C$ , where  $A$ ,  $B$  and  $C$  are

three disjoint subsets of  $V$ . Similarly  $A \perp\!\!\!\perp B$  and  $A \perp\!\!\!\perp B \perp\!\!\!\perp C$  will denote the marginal and the complete independence, respectively, of sub-vectors of  $X$ . There are two Markov properties describing the independence model associated with a bi-directed graph, which we consider in this paper: (a) the global Markov property of Kauermann (1996) and (b) the connected set Markov property by Richardson (2003).

The distribution of the random vector  $X$  satisfies the *global Markov property* for the bi-directed graph  $G$  if for any triple of disjoint sets  $A$ ,  $B$  and  $C$ ,

$$A \perp\!\!\!\perp B \mid V \setminus (A \cup B \cup C) \text{ whenever } A \text{ is separated from } B \text{ by } C \text{ in } G.$$

Instead, the distribution of  $X$  is said to satisfy the *connected set Markov property* if

- (1)  $C_1 \perp\!\!\!\perp \cdots \perp\!\!\!\perp C_r$  whenever  $C_1, \dots, C_r$  are the connected components  
of every disconnected set  $D \in \mathcal{D}$ .

Richardson (2003) proves that the two properties are equivalent; see also Drton & Richardson (2007). Following these authors we define a discrete bi-directed graph model as follows.

**Definition 2.1.** A discrete bi-directed graph model associated with a bi-directed graph  $G = (V, E)$  is a family of discrete joint probability distributions  $p$  for the discrete random vector  $X = (X_v, v \in V)$ , that satisfies the property (1) for  $G$ , i.e. such that, for every disconnected set  $D$  in the graph,

$$p_D(\mathbf{i}_D) = p_{C_1}(\mathbf{i}_{C_1}) \times \cdots \times p_{C_r}(\mathbf{i}_{C_r}),$$

where  $C_1, \dots, C_r$  are the connected components of  $D$ .

If the global Markov property holds then for any pair of not adjacent nodes, the associated random variables are marginally independent. This implication is called the *pairwise Markov property* and it is for discrete variables a necessary but not sufficient condition for the global Markov property. This is in sharp contrast with the family of Gaussian distributions where the two properties are equivalent.

**Example 1.** Here and henceforth we shall use the short forms 34 and 12 to denote the sets  $\{3, 4\}$  and  $\{1, 2\}$ , and so on. The graph of Figure 1(a) is a chain in 4 nodes with disconnected sets

$$\mathcal{D} = \{13, 14, 24, 134, 124\}.$$

Thus,  $D = 13$  has the components  $C_1 = 1$  and  $C_2 = 3$ , while  $D = 134$  can be decomposed into  $C_1 = 1$  and  $C_2 = 34$ . The pairwise Markov property implies  $1 \perp\!\!\!\perp 3$ ,  $1 \perp\!\!\!\perp 4$  and  $2 \perp\!\!\!\perp 4$ , while the connected set Markov property implies further that  $1 \perp\!\!\!\perp 34$  and  $4 \perp\!\!\!\perp 12$ . The global Markov property implies the equivalent set of independence statements  $1 \perp\!\!\!\perp 4$ ,  $2 \perp\!\!\!\perp 4|1$  and  $1 \perp\!\!\!\perp 3|4$ .

Note that the complete list of all marginal independencies implied by a bi-directed graph model is derived from the class  $\mathcal{D}$  of all disconnected sets of the graph.

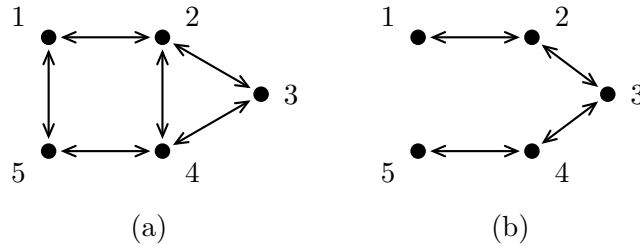


FIGURE 2. Two bi-directed graphs. The independencies implied by the connected set Markov property (or, equivalently, the global Markov property) are: (a)  $1 \perp\!\!\!\perp 34$ ,  $3 \perp\!\!\!\perp 15$  and  $5 \perp\!\!\!\perp 23$ ; (b)  $1 \perp\!\!\!\perp 3 \perp\!\!\!\perp 5$ ,  $1 \perp\!\!\!\perp 345$ ,  $12 \perp\!\!\!\perp 45$  and  $123 \perp\!\!\!\perp 5$ .

**Example 2.** The graph of Figure 2(a) has 7 disconnected sets and thus the associated discrete bi-directed graph model fulfills the independencies

$$1 \perp\!\!\!\perp 3, 1 \perp\!\!\!\perp 4, 2 \perp\!\!\!\perp 5, 3 \perp\!\!\!\perp 5, 1 \perp\!\!\!\perp 34, 5 \perp\!\!\!\perp 23, 3 \perp\!\!\!\perp 15$$

that reduce to  $1 \perp\!\!\!\perp 34$ ,  $3 \perp\!\!\!\perp 15$  and  $5 \perp\!\!\!\perp 23$ , after eliminating redundancies. The discrete model associated with the graph of Figure 2(b) with 16 disconnected subsets satisfies 16 marginal independencies that can be reduced to the four statements

$$1 \perp\!\!\!\perp 3 \perp\!\!\!\perp 5, \quad 1 \perp\!\!\!\perp 345, \quad 12 \perp\!\!\!\perp 45, \quad 123 \perp\!\!\!\perp 5.$$

The stronger condition required by Definition 2.1 implies that in some situations not all marginal independence relations are representable by bi-directed graphs, as the following example shows.

**Example 3.** Consider the data in Table 2, due to Lienert (1970). The variables are 3 symptoms after LSD intake, recorded to be present (level 1) or absent (level 2), and are distortions in affective behavior ( $X_1$ ), distortions in thinking ( $X_2$ ), and dimming of consciousness ( $X_3$ ). As Wermuth (1998) points out, the frequencies in the three marginal tables show that the three symptom pairs are close to independence, but at the same time the variables are not mutual independent as witnessed by the strong three-factor interaction due to the quite distinct conditional odds ratios between  $X_1$  and  $X_2$  at the two levels of  $X_3$ . Thus, in this case, despite three marginal independencies, a discrete bi-directed graph model can represent just one of them, and thus must include at least two edges.

Pearl & Wermuth (1994) studied the Markov equivalence between bi-directed graph models (actually the covariance graphs) and directed acyclic graphs models, i.e. when the two models imply exactly the same conditional independence statements, under their respective global Markov property (for the global Markov property see Lauritzen, 1996). They showed that each bi-directed graph is always Markov equivalent to a directed acyclic graph with additional synthetic latent nodes, after marginalizing over the additional nodes, as exemplified in Figure 1(b, c). Moreover they also give a Markov equivalence result, proving that a bi-directed graph is equivalent to a directed acyclic graph with the same

set of nodes if and only if it contains no 4-chain. Thus, there is no directed acyclic graph which is Markov equivalent to the bi-directed graphs of Figures 1(a), 2(a) or 2(b).

### 3. MARGINAL LOG-LINEAR PARAMETERIZATIONS

Discrete bi-directed graph models may be defined as marginal log-linear models, using complete hierarchical parameterizations as defined by Bergsma & Rudas (2002). In this section we review the basic concepts and we discuss the definitions of the parameters involved. Let  $p(\mathbf{i}) > 0$  be a strictly positive probability distribution of a discrete random vector  $X = (X_v, v \in V)$  and let  $p_M(\mathbf{i}_M)$  be any marginal probability distribution of a sub-vector  $X_M$ ,  $M \subseteq V$ . The marginal probability distribution admits a log-linear expansion

$$\log p_M(\mathbf{i}_M) = \sum_{L \subseteq M} \lambda_L^M(\mathbf{i}_L)$$

where  $\lambda_L^M(\mathbf{i}_L)$  is a function defining the log-linear parameters indexed by the subset  $L$  of  $M$ . The functions  $\lambda_L^M(\mathbf{i}_L)$  are defined by

$$\lambda_L^M(\mathbf{i}_L) = \sum_{A \subseteq L} (-1)^{|L \setminus A|} \log p_M(\mathbf{i}_A, \mathbf{i}_{M \setminus A}^*)$$

where  $\mathbf{i}^* = (1, \dots, 1)$  denotes a baseline cell of the table; see Whittaker (1990) and Lauritzen (1996). The function  $\lambda_L^M(\mathbf{i}_L)$  is zero whenever at least one index in  $\mathbf{i}_L$  is equal to 1. Therefore,  $\lambda_L^M(\mathbf{i}_L)$  defines only  $\prod_{v \in L} (b_v - 1)$  parameters where  $b_v$  is the number of categories of variable  $X_v$ . Due to the constraint on the probabilities, that must sum to one, the parameter  $\lambda_\emptyset^M = \log p(\mathbf{i}_M^*)$  is a function of the others, and can thus be eliminated.

If  $\boldsymbol{\lambda}_L^M$  is the vector containing the parameters  $\lambda_L^M(\mathbf{i}_L)$ , then it can be obtained explicitly using Kronecker products as follows. For any subset  $L$  of  $M$ , let  $\mathbf{C}_{v,L}$  be the matrix

$$\mathbf{C}_{v,L} = \begin{cases} (-\mathbf{1}_{b_v-1} & \mathbf{I}_{b_v-1}) & \text{if } v \in L \\ (1 & \mathbf{0}_{b_v-1}) & \text{if } v \notin L. \end{cases}$$

and let  $\boldsymbol{\pi}^M$  be the  $t_M \times 1$  column vector of the marginal cell probabilities in lexicographic order. Then, the vector of the log-linear parameters  $\boldsymbol{\lambda}_L^M(\mathbf{i}_L)$  is

$$(2) \quad \boldsymbol{\lambda}_L^M = \mathbf{C}_L^M \log \boldsymbol{\pi}^M, \text{ where } \mathbf{C}_L^M = \bigotimes_{v \in M} \mathbf{C}_{v,L}.$$

TABLE 2. *Data by Lienert (1970) concerning symptoms after LSD-intake. OR is the conditional odds-ratio between  $X_1$  and  $X_2$  given  $X_3$ . The frequencies show evidence of pairwise independence, but mutual dependence.*

	$X_3$	1	2		
$X_1$	$X_2$	1	2	1	2
1		21	5	4	16
2		2	13	11	1
OR		27.3		0.023	

For a discussion of the technique of building all log-linear parameters based on Kronecker products see Wermuth & Cox (1992). The coding used in this paper corresponds to their indicator coding, and gives the parameters used for example by the program GLIM.

A marginal log-linear parameterization of the probability distribution  $p(\mathbf{i})$  is obtained by combining the log-linear parameters  $\boldsymbol{\lambda}_L^M$  for many different marginal probability distributions. The general theory is developed in Bergsma & Rudas (2002) and is summarized below.

**Definition 3.1.** *Let  $\mathcal{M} = (M_1, \dots, M_s)$  be an ordered sequence of margins of interest, and, for each  $M_j$ ,  $j = 1, \dots, s$ , let  $\mathcal{L}_j$  be the collection of sets  $L$  for which  $\boldsymbol{\lambda}_L^{M_j}$  is defined with equation (2). Then,  $(\boldsymbol{\lambda}_L^{M_j})$  is said to be a hierarchical and complete marginal log-linear parameterization for  $p(\mathbf{i})$  if (i) the sequence  $M_1, \dots, M_s$  is non-decreasing; (ii) the last margin is  $M_s = V$ ; (iii) the sets defining the log-linear parameters in each margin are:*

$$\mathcal{L}_1 = \mathcal{P}_0(M_1), \text{ and } \mathcal{L}_j = \mathcal{P}_0(M_j) \setminus \bigcup_{h=1}^{j-1} \mathcal{L}_h, \text{ for } j > 1,$$

where  $\mathcal{P}_0(M_j)$  denotes the collection of all non-empty sets of  $M_j$ .

The parameterization is called hierarchical because it is generated by a non-decreasing sequence  $\mathcal{M}$ , and complete because it defines all possible log-linear parameters terms, each within one and only one marginal table. Notice that the parameterization is associated uniquely to a particular sequence  $\mathcal{M}$  of margins. Thus, a different (still non-decreasing) ordering of the sequence induces a different parameterization; see the examples in Section 4.2.

The above construction defines a map from the simplex  $\Delta_V$  of the strictly positive distributions  $p(\mathbf{i})$  of the discrete random vector  $X$  into the set  $\Lambda$  of possible values for the whole vector of the marginal log-linear parameters  $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_L^{M_j})$ , with  $j = 1, \dots, s$  and  $L \in \mathcal{L}_j$ . The following general result shows that a complete hierarchical marginal log-linear model defines a proper parameterization.

**Proposition 1.** *(Bergsma & Rudas, 2002) The map  $\Delta_V \rightarrow \Lambda \subseteq \mathbf{R}^{t-1}$  defined by a complete and hierarchical marginal log-linear parameterization is a diffeomorphism.*

The parameters  $\boldsymbol{\lambda}$  can be written in matrix form

$$\boldsymbol{\lambda} = \mathbf{C} \log(\mathbf{T}\boldsymbol{\pi})$$

where  $\boldsymbol{\pi}$  is the  $t \times 1$  vector of all the cell probabilities in lexicographical order,  $\mathbf{T}$  is a  $m \times t$  marginalization matrix such that

$$\mathbf{T}\boldsymbol{\pi} = \begin{pmatrix} \boldsymbol{\pi}^{M_1} \\ \vdots \\ \boldsymbol{\pi}^{M_s} \end{pmatrix}$$

and  $\mathbf{C} = \text{diag}(\mathbf{C}_L^M)$  is a  $t-1 \times m$  block diagonal matrix, with  $m = \sum_{j=1}^s |\mathcal{I}_{M_j}|$ . For a discussion of algorithms for computing the matrices  $\mathbf{C}$  and  $\mathbf{T}$  see Bartolucci *et al.* (2007), that generalize the approach by Bergsma & Rudas (2002) to logits and higher order effects of global and continuation type, suitable with ordinal data.



The log-linear parameterization and the multivariate logistic transformation represent two special cases of marginal log-linear models. The standard log-linear parameters are generated by  $\mathcal{M} = \{V\}$ . They will be denoted by  $\theta_L = \lambda_L^V$  for  $L \in \mathcal{P}_0(V)$  and the whole vector of parameters by  $\theta$ . The parameter space coincides with  $\mathbf{R}^{t-1}$  and the map from  $\pi$  to  $\theta$  admits an inverse in closed form, provided that  $\pi > 0$ . The multivariate logistic parameters Glonek & McCullagh (1995) are generated by  $\mathcal{M} = \mathcal{P}_0(V)$ , in any non-decreasing order. They will be denoted by  $\eta^M = \lambda_M^M$ , with  $\eta$  representing the whole vector. Thus the parameters  $\eta^M$  correspond to the highest order log-linear parameters within each marginal table  $\mathcal{I}_M$ , for each nonempty set  $M \subseteq V$ . The parameter space is in general a strict subset of  $\mathbf{R}^{t-1}$ , except when the number of variables is  $d = 2$ . In general there is no closed form inverse transforming back  $\eta$  into  $\pi$ . The inverse operation however may be accomplished using for example the iterative proportional fitting algorithm.

Thus, while the log-linear parameters  $\theta$  are always variation independent and for any  $\theta$  in  $\mathbf{R}^{t-1}$  there is a unique associated joint probability distribution  $\pi$ , instead the multivariate logistic parameters are never variation independent, for  $d > 2$ . Thus there are vectors  $\eta$  in  $\mathbf{R}^{t-1}$  that are not compatible with any joint probability distribution  $\pi$ . The latter assertion is also implied by a further result by Bergsma & Rudas (2002) which proves that the hierarchical and complete marginal log-linear parameterization generated by a sequence  $\mathcal{M}$  is variation independent if and only if  $\mathcal{M}$  satisfies a property called *ordered decomposability*. A sequence of arbitrary subsets of  $V$  is said to be ordered decomposable if it has at most two elements or if there is an ordering  $M_1, \dots, M_s$  of its elements, such that  $M_i \not\subseteq M_j$  if  $i > j$  and, for  $k = 3, \dots, s$ , the maximal elements (i.e. those not contained in any other sets) of  $\{M_1, \dots, M_k\}$  form a decomposable set. For further details and examples about ordered decomposability see Rudas & Bergsma (2004). More properties of the two parameterizations  $\theta$  and  $\eta$ , connected to graphical models, will be described in the next Section 4.

#### 4. PARAMETERIZATIONS OF DISCRETE BI-DIRECTED GRAPH MODELS

We suggest now two different marginal log-linear parameterizations of discrete bi-directed graph models, and we compare advantages and shortcomings.

**4.1. Multivariate logistic parameterization.** It is known that the complete independence of two sub-vectors  $X_A, X_B$  of the random vector  $X$  is equivalent to a set of zero restrictions on multivariate logistic parameters.

**Lemma 1.** (Kauermann (1997), Lemma 1). *If  $\{A, B\}$  is a partition of  $V$  and  $\eta = (\eta^M), M \in \mathcal{P}_0(V)$  is the multivariate logistic parameterization, then*

$$A \perp\!\!\!\perp B \iff \eta^M = \mathbf{0} \quad \text{for all } M \in \mathcal{Q}$$

where  $\mathcal{Q} = \{M \subseteq A \cup B : M \cap A \neq \emptyset, M \cap B \neq \emptyset\}$ .

We generalize this result to complete independence of more than two random vectors. Given a partition  $\{C_1, \dots, C_r\}$  of a set  $D \subseteq V$ , we define

$$\mathcal{Q}(C_1, \dots, C_r) = \mathcal{P}(\bigcup_{i=1}^r C_i) \setminus \bigcup_{i=1}^r \mathcal{P}(C_i).$$

This is the set of all subsets of  $D$  not completely contained in a single class, i.e. containing elements coming from at least two classes of the partition. With this notation, the set  $\mathcal{Q}$  of Lemma 1 may be denoted by  $\mathcal{Q}(A, B)$ . Then we have the following result.

**Proposition 2.** *Let  $X = (X_v), v \in V$ , be the discrete random vector with multivariate logistic parameterization  $\boldsymbol{\eta} = (\boldsymbol{\eta}^M), M \in \mathcal{P}_0(V)$ . If  $D \subseteq V$  is partitioned into the classes  $\{C_1, \dots, C_r\}$  then*

$$C_1 \perp\!\!\!\perp \dots \perp\!\!\!\perp C_r \iff \text{for all } M \in \mathcal{Q}(C_1, \dots, C_r) : \quad \boldsymbol{\eta}^M = \mathbf{0}.$$

*Proof.* First, use the shorthand notations  $\mathcal{Q}$  to denote the set  $\mathcal{Q}(C_1, \dots, C_r)$  and  $\mathcal{Q}_i$  to denote the set  $\mathcal{Q}(C_i, C_{-i})$ ,  $i = 1, \dots, r$ , where  $C_{-i} = D \setminus C_i$ . In fact, since  $\mathcal{Q}_i \subseteq \mathcal{Q}$ , then  $\bigcup_{i=1}^r \mathcal{Q}_i \subseteq \mathcal{Q}$ . Conversely, for any  $M \in \mathcal{Q}$  there is always a class  $C_i$  such that  $C_i \not\subseteq M$ , and hence, by definition,  $M \in \mathcal{Q}_i$ . Hence, for every  $M \in \mathcal{Q}$ ,  $M \in \bigcup_{i=1}^r \mathcal{Q}_i$  and thus  $\mathcal{Q} \subseteq \bigcup_{i=1}^r \mathcal{Q}_i$ . Then, the complete independence  $C_1 \perp\!\!\!\perp \dots \perp\!\!\!\perp C_r$  is equivalent to  $C_i \perp\!\!\!\perp C_{-i}$  for all  $i = 1, \dots, r$ . By Lemma 1, applied to the sub-vector  $X_D$ , each independence  $C_i \perp\!\!\!\perp C_{-i}$  is equivalent to the restriction  $\boldsymbol{\eta}^M = \mathbf{0}$  for  $M \in \mathcal{Q}_i$  and the parameters  $\boldsymbol{\eta}^M$  are identical to the corresponding multivariate logistic parameters for the full random vector  $X_V$ . Thus, the complete independence  $C_1 \perp\!\!\!\perp \dots \perp\!\!\!\perp C_r$  is equivalent to  $\boldsymbol{\eta}^M = \mathbf{0}$  for  $M \in \mathcal{Q}_i$ ,  $i = 1, \dots, r$ , i.e. for  $M \in \bigcup_{i=1}^r \mathcal{Q}_i = \mathcal{Q}$ .  $\square$

Proposition 2 implies that a statement of complete independence  $C_1 \perp\!\!\!\perp \dots \perp\!\!\!\perp C_r$  is equivalent to a set of zero constraints on the multivariate logistic parameters. The following result explains how the constraints must be chosen in order to satisfy all the independencies required by the Definition 2.1 of a bi-directed graph model.

**Proposition 3.** *Given a bi-directed graph  $G = (V, E)$ , the discrete bi-directed graph model associated with  $G$  is defined by the set of strictly positive discrete probability distributions with multivariate logistic parameters  $\boldsymbol{\eta} = (\boldsymbol{\eta}^M), M \in \mathcal{P}_0(V)$ , such that*

$$\boldsymbol{\eta}^M = \mathbf{0} \text{ for every } M \in \mathcal{D},$$

where  $\mathcal{D}$  is the set of all disconnected sets of nodes in the graph  $G$ .

*Proof.* Given a set  $D \in \mathcal{D}$ , denote its connected components by  $\{C_1, \dots, C_r\}$  and by  $\mathcal{Q}_D$  the set  $\mathcal{Q}(C_1, \dots, C_r)$ . First, we prove that  $\mathcal{D} = \bigcup_{D \in \mathcal{D}} \mathcal{Q}_D$ . In fact, for any  $D \in \mathcal{D}$ ,  $\mathcal{Q}_D \subseteq \mathcal{D}$  because it is a class of disconnected subsets of  $D$ . Thus,  $\bigcup_{D \in \mathcal{D}} \mathcal{Q}_D \subseteq \mathcal{D}$ . Conversely, if  $D \in \mathcal{D}$ , then  $D \in \mathcal{Q}_D$  and thus  $\mathcal{D} \subseteq \bigcup_{D \in \mathcal{D}} \mathcal{Q}_D$ . By Definition 2.1, the independence  $C_1 \perp\!\!\!\perp \dots \perp\!\!\!\perp C_r$  is implied for each disconnected set  $D$  with connected components  $C_1, \dots, C_r$ . By Proposition 2, this is equivalent to the zero restrictions on the multivariate logistic parameters

$$\boldsymbol{\eta}^M = \mathbf{0}, \text{ for all } M \in \mathcal{Q}_D, \quad D \in \mathcal{D}$$

i.e. for all  $M \in \bigcup_{D \in \mathcal{D}} \mathcal{Q}_D = \mathcal{D}$ .  $\square$

A consequence of Proposition 3 is that all possible discrete bi-directed graphical models can be identified within the multivariate logistic parametrization under the zero constraints associated with the disconnected sets.

TABLE 3. *Comparison between two parameterization of the discrete chordless 4-chain model of Figure 1(a): ( $\boldsymbol{\eta}$ ) with bi-directed edges; ( $\boldsymbol{\theta}$ ) with undirected edges.*

Terms	1	2	3	4	12	13	14	23	24	34	123	124	134	234	1234
$\boldsymbol{\eta}$	$\boldsymbol{\eta}^1$	$\boldsymbol{\eta}^2$	$\boldsymbol{\eta}^3$	$\boldsymbol{\eta}^4$	$\boldsymbol{\eta}^{12}$	$\mathbf{0}$	$\mathbf{0}$	$\boldsymbol{\eta}^{23}$	$\mathbf{0}$	$\boldsymbol{\eta}^{34}$	$\boldsymbol{\eta}^{123}$	$\mathbf{0}$	$\mathbf{0}$	$\boldsymbol{\eta}^{234}$	$\boldsymbol{\eta}^{1234}$
$\boldsymbol{\theta}$	$\boldsymbol{\theta}_1$	$\boldsymbol{\theta}_2$	$\boldsymbol{\theta}_3$	$\boldsymbol{\theta}_4$	$\boldsymbol{\theta}_{12}$	$\mathbf{0}$	$\mathbf{0}$	$\boldsymbol{\theta}_{23}$	$\mathbf{0}$	$\boldsymbol{\theta}_{34}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$

**Example 4.** The discrete model associated with the chordless 4-chain of Figure 1(a) is defined by the multivariate logistic parameters shown in Table 3, first row. There are 5 zero constraints on the highest-order log-linear parameters of the tables 13, 14, 24, 124 134. There are three nonzero two-factor marginal log-linear parameter  $\boldsymbol{\eta}^{ij}$  associated with the edges of the graph that may be interpreted as sets of marginal association coefficients between the involved variables, based on the chosen contrasts. Consider now the reduced model resulting after dropping the edge  $2 \leftrightarrow 3$  and implying the independence  $12 \perp\!\!\!\perp 34$ . This model can be obtained, within the same parameterization, by the additional zero constraints on  $\boldsymbol{\eta}^{23}, \boldsymbol{\eta}^{123}, \boldsymbol{\eta}^{234}$  and  $\boldsymbol{\eta}^{1234}$ .

While the parameters are in general not variation independent, they satisfy the upward compatibility property, because they have the same meaning across different marginal distributions. Using this property, we can prove the following result concerning the effect of marginalization over a subset  $A$  of the variables. Let  $G_A = (A, E_A)$  be the subgraph induced by  $A$ , and let  $\mathcal{D}_A$  be the set of all disconnected sets of  $G_A$ .

**Proposition 4.** *If a discrete probability distribution  $p(\mathbf{i})$  for  $\mathbf{i} \in \mathcal{I}_V$  satisfies a bi-directed graph model defined by the graph  $G = (V, E)$  then the marginal distribution  $p_A(\mathbf{i}_A)$  over  $A \subseteq V$  satisfies the bi-directed graph model defined by  $G_A = (A, E_A)$  and its multivariate logistic parameters are  $\boldsymbol{\eta} = (\boldsymbol{\eta}^M), M \in \mathcal{P}_0(A)$  with constraints  $\boldsymbol{\eta}^M = \mathbf{0}$ , for  $M \in \mathcal{D}_A$ .*

*Proof.* After marginalization over  $A$ , the multivariate logistic parameters associated with  $p_A(\mathbf{i}_A)$ , by the property of upward compatibility, are  $(\boldsymbol{\eta}^M, M \in \mathcal{P}_0(A))$ . Some of these parameters are zero by the constraints implied by the original bi-directed graph model, i.e.  $\boldsymbol{\eta}^M = \mathbf{0}$ , for  $M \in \mathcal{D} \cap \mathcal{P}_0(A)$ . The result is proved by showing that  $\mathcal{D} \cap \mathcal{P}_0(A) = \mathcal{D}_A$ . First, we note that if  $D \subseteq A \subseteq V$ , then the graph  $G_D = (D, E_D)$  with edges  $E_D = (D \times D) \cap E = (D \times D) \cap E_A$  is a subgraph of both  $G_A$  and  $G$ . Thus, if  $D \subseteq A$  and  $D \in \mathcal{D}$  then the induced subgraph  $G_D$  is disconnected and being also a subgraph of  $G_A$  then  $D$  is also a disconnected set of  $G_A$ . Thus  $\mathcal{D} \cap \mathcal{P}_0(A) \subseteq \mathcal{D}_A$ . Conversely, if  $D$  is a disconnected set of  $G_A$ , then the subgraph  $G_D$  is disconnected, and being a subgraph of  $G$ , then  $D$  is also a disconnected set of  $G$ . Thus  $\mathcal{D}_A \subseteq \mathcal{D} \cap \mathcal{P}_0(A)$ , and the result follows.  $\square$

Discrete bi-directed graph models in the multivariate logistic parameterization can be compared with discrete log-linear graphical models represented by undirected graphs with the same skeleton (i.e. with the same set  $E$ ). To facilitate the comparison we state the following well-known result, following from the Hammersley and Clifford theorem, (see Lauritzen, 1996, p. 36), which is the undirected graph model counterpart of Proposition 3.

**Proposition 5.** *Given an undirected graph  $G = (V, E)$ , a discrete graphical log-linear model associated with  $G$  is defined by the set of strictly positive discrete probability distributions with log-linear parameters  $\boldsymbol{\theta} = (\boldsymbol{\theta}_L, L \in \mathcal{P}_0(V))$ , such that*

$$\boldsymbol{\theta}_L = \mathbf{0} \text{ for every } L \in \mathcal{N},$$

where  $\mathcal{N}$  is the set of all incomplete subsets of nodes in the graph  $G$ .

The set  $\mathcal{D}$  of all disconnected sets of a graph  $G$  is included in the set  $\mathcal{N}$  of the incomplete sets, and therefore the number of zero restrictions of the undirected graph models is always higher than the number of zero restrictions of the bi-directed graph models with the same skeleton, (see Drton & Richardson, 2007).

**Example 5.** A discrete undirected graph model for the 4-chain implies the independencies  $12 \perp\!\!\!\perp 4|3$  and  $1 \perp\!\!\!\perp 34|2$  and is defined by zero constraints on 8 log-linear parameters  $\boldsymbol{\theta}_L$ , shown in Table 3, second row. Also, Proposition 5 implies that in the discrete undirected graph model the general hierarchy principle holds, i.e. if a particular log-linear term is zero then all higher terms containing the same set of subscripts are also set to zero. On the contrary, by Proposition 3, in the multivariate logistic parameterization of the bi-directed graph model the hierarchy principle is violated because a superset of a disconnected set may be connected. Thus, for instance in the example shown in Table 3 there are zero pairwise associations, like  $\boldsymbol{\eta}^{13} = \mathbf{0}$ , but nonzero higher order log-linear parameters like  $\boldsymbol{\eta}^{123} \neq \mathbf{0}$  and  $\boldsymbol{\eta}^{1234} \neq \mathbf{0}$ .

**4.2. The disconnected sets parameterization.** We discuss now another marginal log-linear parameterization that can represent the independence constraints implied by any discrete bi-directed graph model, but involving only those marginal tables which are needed. This parameterization defines the log-linear parameters within the margins associated with the disconnected sets of the graph defining the model. Specifically, given a discrete graph model with a graph  $G$ , we arbitrarily order the disconnected sets of the graph to yield a non-decreasing sequence  $(D_1, \dots, D_s)$  such that  $D_k \not\supseteq D_{k+1}$  for  $k = 1, \dots, s-1$ . Then, the *disconnected set parameterization* of the discrete bi-directed graph model associated with  $G$ , is the hierarchical and complete marginal log-linear parameterization  $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_L^{M_j})$  generated, following Definition 3.1, by the sequence of margins

$$(3) \quad \mathcal{M}_G = \begin{cases} (D_1, \dots, D_s) & \text{if } D_s = V \\ (D_1, \dots, D_s, V) & \text{otherwise.} \end{cases}$$

This parameterization contains by definition the log-linear parameters  $\boldsymbol{\lambda}_D^D = \boldsymbol{\eta}^D$  for every disconnected set  $D$  and thus can define the independence model by the same constraints of Proposition 3.

**Proposition 6.** *Given a bi-directed graph  $G = (V, E)$ , the discrete bi-directed graph model associated with  $G$  is defined by the set of strictly positive discrete probability distributions with a disconnected set parameterization  $(\boldsymbol{\lambda}_L^{M_j})$ , such that*

$$\boldsymbol{\lambda}_{M_j}^{M_j} = \mathbf{0} \text{ for every } M_j \in \mathcal{D},$$

TABLE 4. *Comparison of three parameterizations for the bi-directed graph model  $G$  of Figure 1(a). One-factor log-linear parameters are omitted. The columns of parameters to be constrained to zero have a boldfaced label.*

Terms	12	<b>13</b>	<b>14</b>	23	<b>24</b>	34	123	<b>124</b>	<b>134</b>	234	1234
$\eta$	$\eta^{12}$	$\eta^{13}$	$\eta^{14}$	$\eta^{23}$	$\eta^{24}$	$\eta^{34}$	$\eta^{123}$	$\eta^{124}$	$\eta^{134}$	$\eta^{234}$	$\eta^{1234}$
$\mathcal{M}_G$	$\lambda_{12}^{124}$	$\lambda_{13}^{13}$	$\lambda_{14}^{14}$	$\lambda_{23}^{1234}$	$\lambda_{24}^{24}$	$\lambda_{34}^{134}$	$\lambda_{123}^{1234}$	$\lambda_{124}^{124}$	$\lambda_{134}^{134}$	$\lambda_{234}^{1234}$	$\lambda_{1234}^{1234}$
$\mathcal{M}'_G$	$\lambda_{12}^{124}$	$\lambda_{13}^{134}$	$\lambda_{14}^{14}$	$\lambda_{23}^{1234}$	$\lambda_{24}^{124}$	$\lambda_{34}^{134}$	$\lambda_{123}^{1234}$	$\lambda_{124}^{124}$	$\lambda_{134}^{134}$	$\lambda_{234}^{1234}$	$\lambda_{1234}^{1234}$

where  $\mathcal{D}$  is the class of all disconnected sets for  $G$ . Moreover, the constraints are independent of the ordering chosen to define  $\mathcal{M}_G$ .

*Proof.* The disconnected set parameterization defined by the sequence (3), contains the parameters  $\lambda_L^D$ , with  $D \in \mathcal{D}$ . By Definition 3.1,  $\mathcal{L}_j$ ,  $j = 1, \dots, s$  always contains the set  $D$  itself. This happens whatever ordering is used to define  $\mathcal{M}_G$ . Thus the parameterization always includes  $\lambda_D^D = \eta^D$ , for every  $D \in \mathcal{D}$  and it is possible to impose the constraints  $\eta^D = \mathbf{0}$  for every  $D \in \mathcal{D}$  and the result follows by Proposition 3.  $\square$

While the constrained parameters defining the bi-directed graph model are actually the same as the multivariate logistic parameterization, the other unconstrained log-linear parameters are defined in larger marginal tables, and thus have a different interpretation. An important difference is that the disconnected set parameterization is tied to the specific graph  $G$  defining the model. This implies that it is not possible to define every bi-directed graph model within the same disconnected set parameterization. A different model  $G$  implies a different sequence  $\mathcal{M}_G$  of disconnected sets and thus a different list of log-linear parameters.

**Example 6.** For the chordless 4-chain graph of Figure 1(a), there are several possible orderings of the 5 disconnected sets  $\mathcal{D} = \{13, 14, 24, 134, 124\}$ . The discrete bi-directed graph model is defined by choosing for example

$$\mathcal{M}_G = (13, 14, 24, 134, 124, 1234),$$

and by constraining the marginal log-linear parameters  $\lambda_D^D = \mathbf{0}$  for  $D \in \mathcal{D}$ . The unconstrained parameters differ from the multivariate logistic ones. For example the two-factor log-linear parameters between  $X_1$  and  $X_2$ ,  $\lambda_{12}^{124}$ , are defined within the marginal table 124 instead of the marginal table 12. A detailed comparison between the parameters is reported in the first two rows of the Table 3.

The previous example shows that we can collect the log-linear parameters into a reduced number of marginal tables. An alternative selection of marginal tables could be chosen in order to fulfill the conditional independencies implied by the global Markov property. We will describe the method in the special case of the chordless 4-chain graph. It is conjectured that a general variation independent parameterization does not exists for all bi-directed graphs, but the definition of a sub-class admitting such a parameterization is still an open problem.

**Example 7.** In Example 1 we stated that, for the bi-directed 4-chain graph of Figure 1(a), the global Markov property implies the conditional independencies  $1 \perp\!\!\!\perp 4$ ,  $2 \perp\!\!\!\perp 4|1$  and  $1 \perp\!\!\!\perp 3|4$ . Thus, the relevant margins can be collected in the sequence

$$\mathcal{M}'_G = (14, 134, 124, 1234)$$

where the first three allow the definition of the conditional independencies and the last one serves as completion of the parameterization. The complete hierarchical parameterization generated by  $\mathcal{M}'_G$  is slightly different from that generated by  $\mathcal{M}_G$ , see Table 4, third row, but with the 5 zero constraints on the higher level log-linear parameters within each margin, we obtain the required independencies

$$1 \perp\!\!\!\perp 4 \iff \lambda_{14}^{14} = \mathbf{0} \quad 2 \perp\!\!\!\perp 4|1 \iff \begin{cases} \lambda_{24}^{124} = \mathbf{0} \\ \lambda_{124}^{124} = \mathbf{0} \end{cases} \quad 1 \perp\!\!\!\perp 3|4 \iff \begin{cases} \lambda_{13}^{134} = \mathbf{0} \\ \lambda_{134}^{134} = \mathbf{0}. \end{cases}$$

Note that these independencies can also be represented by a chain graph with two components,  $\{1, 4\}$  and  $\{2, 3\}$ , under the alternative Markov property, (see Andersson *et al.*, 2001). The associated discrete model is interpreted as a system of seemingly unrelated regressions, with two joint responses  $X_2$  and  $X_3$ . In this context the associations of interest are the effect parameters between every response and each explanatory variable conditional on the remaining explanatory variable, i.e.  $\lambda_{12}^{124}$ ,  $\lambda_{24}^{124}$ ,  $\lambda_{13}^{134}$  and  $\lambda_{34}^{134}$ , and the marginal association parameters between the explanatory variables,  $\lambda_{14}^{14}$ . By relaxing the constraint  $\lambda_{14}^{14} = \mathbf{0}$  we obtain a discrete chain graph model with two complete chain components, under the alternative Markov property.

In the comparison between different parameterizations also the property of variation independence may be relevant. Following Bergsma & Rudas (2002), given a discrete bi-directed graph model, there is a variation independent parameterization if there is at least a sequence  $\mathcal{M}_G$  which is ordered decomposable. This property is quite relevant because the lack of variation independence may make the separate interpretation of the parameters misleading.

**Example 8.** In the previous example both the parameterizations based on  $\mathcal{M}_G$  and  $\mathcal{M}'_G$  are variation independent (unlike the multivariate logistic parameterization) because the sequences of margins are both ordered decomposable. Consider instead the bi-directed graph in Figure 2(a). Two possible disconnected set parameterizations of the discrete model may be based for example on

$$\begin{aligned} \mathcal{M}_G &= (13, 14, 25, 35, 134, 135, 235, 12345), \\ \mathcal{M}'_G &= (13, 35, 135, 14, 25, 134, 235, 12345). \end{aligned}$$

with the constraints  $\lambda_D^D = \mathbf{0}$  for any disconnected set  $D$ . In this case we can verify that only the sequence  $\mathcal{M}'_G$  is ordered decomposable and thus implies variation independent parameters.

## 5. MAXIMUM LIKELIHOOD ESTIMATION OF DISCRETE BI-DIRECTED GRAPH MODELS

We study now the maximum likelihood estimation of the discrete bi-directed graph models under any of the parameterizations previously discussed. Assuming a multinomial sampling scheme with sample size  $N$ , each individual falls in a cell  $\mathbf{i}$  of the given contingency table  $\mathcal{I}_V$  with probability  $p(\mathbf{i}) > 0$ . Let  $n(\mathbf{i})$  be the cell count and  $\mathbf{n} = (n(\mathbf{i}), \mathbf{i} \in \mathcal{I}_V)$ , be a  $t \times 1$  vector. Thus,  $\mathbf{n}$  has a multinomial distribution with parameters  $N$  and  $\boldsymbol{\pi}$ . If  $\boldsymbol{\mu} = N\boldsymbol{\pi} > \mathbf{0}$  is the expected value of  $\mathbf{n}$  and  $\boldsymbol{\omega} = \log \boldsymbol{\mu}$ , then for any appropriate marginal log-linear parameterization  $\boldsymbol{\lambda}$  we have  $\boldsymbol{\lambda} = \mathbf{C} \log(\mathbf{T}\boldsymbol{\pi}) = \mathbf{C} \log(\mathbf{T} \exp(\boldsymbol{\omega}))$  because the contrasts of marginal probabilities are equal to the contrasts of expected counts. Given a discrete bi-directed graph model defined by the graph  $G = (V, E)$ , if  $\boldsymbol{\lambda}$  is defined either by the multivariate logistic parameterization or by the disconnected set parameterization, we can always split  $\boldsymbol{\lambda}$  in two components  $\boldsymbol{\lambda}_{\mathcal{D}}$  and  $\boldsymbol{\lambda}_{\mathcal{C}}$  indexed by the disconnected sets  $\mathcal{D}$  and by the connected sets  $\mathcal{C}$  of the graph, respectively. If  $\mathbf{C}_{\mathcal{D}}$  is a sub-matrix of the contrast matrix  $\mathbf{C}$ , obtained by selecting the rows associated with the disconnected sets of the graph  $G$ ,

$$\boldsymbol{\lambda}_{\mathcal{D}} = \mathbf{C}_{\mathcal{D}} \log(\mathbf{T} \exp(\boldsymbol{\omega})) = \mathbf{h}(\boldsymbol{\omega})$$

where  $\mathbf{C}_{\mathcal{D}}$  has dimensions  $q \times v$  with  $q = \sum_{D \in \mathcal{D}} \prod_{v \in D} (b_v - 1)$ . Thus, the kernel of the log-likelihood function of the discrete bi-directed graph model is defined by

$$(4) \quad l(\boldsymbol{\omega}; \mathbf{n}) = \mathbf{n}^T \boldsymbol{\omega} - \mathbf{1}^T \exp(\boldsymbol{\omega}), \quad \boldsymbol{\omega} \in \Omega_{BG},$$

with

$$\Omega_{BG} = \{\boldsymbol{\omega} \in \mathbf{R}^t : \mathbf{h}(\boldsymbol{\omega}) = \mathbf{0}, \quad \mathbf{1}^T \exp(\boldsymbol{\omega}) = N\}.$$

Note that (4) defines a curved exponential family model as the set  $\Omega_{BG}$  is a smooth manifold in the space  $\mathbf{R}^t$  of the canonical parameters  $\boldsymbol{\mu}$ . Maximum likelihood estimation is a constrained optimization problem and the maximum likelihood estimate is a saddle point of the Lagrangian log-likelihood

$$\ell(\boldsymbol{\omega}, \boldsymbol{\tau}) = \mathbf{n}^T \boldsymbol{\omega} - \mathbf{1}^T \exp(\boldsymbol{\omega}) + \boldsymbol{\tau}^T \mathbf{h}(\boldsymbol{\omega})$$

where  $\boldsymbol{\tau}$  is a  $q \times 1$  vector of unknown Lagrange multipliers. To solve the equations we propose an iterative procedure inspired by Aitchison & Silvey (1958), Lang (1996) and Bergsma (1997). Define first

$$\boldsymbol{\xi} = \begin{pmatrix} \boldsymbol{\omega} \\ \boldsymbol{\tau} \end{pmatrix}, \quad \mathbf{f}(\boldsymbol{\xi}) = \frac{\partial \ell}{\partial \boldsymbol{\xi}} = \begin{pmatrix} \mathbf{f}_{\boldsymbol{\omega}} \\ \mathbf{f}_{\boldsymbol{\tau}} \end{pmatrix} \quad \mathbf{F}(\boldsymbol{\xi}) = -E \left( \frac{\partial^2 \ell}{\partial \boldsymbol{\xi} \partial \boldsymbol{\xi}^T} \right) = \begin{pmatrix} \mathbf{F}_{\boldsymbol{\omega}\boldsymbol{\omega}} & \mathbf{F}_{\boldsymbol{\omega}\boldsymbol{\tau}} \\ \cdot & \mathbf{F}_{\boldsymbol{\tau}\boldsymbol{\tau}} \end{pmatrix},$$

where the dot is a shortcut to denote a symmetric sub-matrix. Differentiating the Lagrangian with respect to  $\boldsymbol{\omega}$  and  $\boldsymbol{\tau}$  and equating the result to zero we obtain

$$(5) \quad \begin{pmatrix} \mathbf{f}_{\boldsymbol{\omega}} \\ \mathbf{f}_{\boldsymbol{\tau}} \end{pmatrix} = \begin{pmatrix} \mathbf{e} + \mathbf{H}\boldsymbol{\tau} \\ \mathbf{h}(\boldsymbol{\omega}) \end{pmatrix} = \mathbf{0}$$

where  $\mathbf{e} = \partial l / \partial \boldsymbol{\omega} = \mathbf{n} - \boldsymbol{\mu}$ ,  $\mathbf{H} = \partial \mathbf{h} / \partial \boldsymbol{\omega}^T = \mathbf{D}_{\boldsymbol{\mu}} \mathbf{T}^T \mathbf{D}_{T\boldsymbol{\mu}}^{-1} \mathbf{C}_{\mathcal{D}}^T$  and  $\mathbf{D}_{T\boldsymbol{\mu}}$  and  $\mathbf{D}_{\boldsymbol{\mu}}$  are diagonal matrices, with nonzero elements  $\mathbf{T}\boldsymbol{\mu}$  and  $\boldsymbol{\mu}$ , respectively.

Let  $\hat{\boldsymbol{\omega}}$  be a local maximum of the likelihood subject to the constraint  $\mathbf{h}(\boldsymbol{\omega}) = \mathbf{0}$ . A classical result (Bertsekas, 1982) is that if  $\mathbf{H}$  is of full column rank at  $\hat{\boldsymbol{\omega}}$ , there is a unique  $\hat{\boldsymbol{\tau}}$  such that  $\ell(\hat{\boldsymbol{\omega}}, \hat{\boldsymbol{\tau}}) = \mathbf{0}$ . In the sequel, it is assumed that the maximum likelihood estimate

$\hat{\omega}$  is a solution to the equation (5). Note that the constraint  $\mathbf{1}^T \boldsymbol{\mu} = \mathbf{1}^T \mathbf{n}$  is automatically satisfied as it can be verified that  $\mathbf{H}^T \mathbf{1} = \mathbf{0}$  and thus from (5) it follows that  $\mathbf{1}^T \mathbf{e} = \mathbf{0}$ .

Aitchison and Silvey propose a Fisher score like updating function

$$(6) \quad \boldsymbol{\xi}^{(k+1)} = \mathbf{u}(\boldsymbol{\xi}^{(k)}), \text{ with } \mathbf{u}(\boldsymbol{\xi}) = \boldsymbol{\xi} + \mathbf{F}^{-1}(\boldsymbol{\xi}) \mathbf{f}(\boldsymbol{\xi}),$$

yielding the estimate  $\boldsymbol{\xi}^{(k+1)}$  at cycle  $k+1$  from that at cycle  $k$ . As the algorithm does not always converge when starting estimates are not close enough to  $\hat{\omega}$ , it is necessary to introduce a step size into the updating equation. The standard approach to choosing a step size in optimization problems is to use a value for which the objective function to be maximized increases. However, since in this case we are looking for a saddle point of the Lagrangian likelihood  $\ell$ , we need to adjust the standard strategy. First, the matrix  $\mathbf{F}$  has a special structure with  $\mathbf{F}_{\omega\omega} = \mathbf{D}_\mu$ ,  $\mathbf{F}_{\omega\tau} = -\mathbf{H}$  and  $\mathbf{F}_{\tau\tau} = \mathbf{0}$ . Thus, indicating the sub-matrices of  $\mathbf{F}^{-1}$  by superscripts, we have  $\mathbf{F}_{\tau\omega} \mathbf{F}^{\omega\tau} = \mathbf{I}$  and  $\mathbf{F}^{\omega\omega} \mathbf{F}_{\omega\tau} = \mathbf{0}$ . Thus the updating function  $\mathbf{u}(\boldsymbol{\xi})$  of (6) can be rewritten as follows

$$\mathbf{u}_\omega(\boldsymbol{\omega}) = \boldsymbol{\omega} + \mathbf{F}^{\omega\omega} \mathbf{e} + \mathbf{F}^{\omega\tau} h(\boldsymbol{\omega}), \quad \mathbf{u}_\tau(\boldsymbol{\omega}) = \mathbf{F}^{\tau\omega} \mathbf{e} + \mathbf{F}^{\tau\tau} h(\boldsymbol{\omega}),$$

neither of which is a function of  $\boldsymbol{\tau}$ . As the updating of the Lagrange multipliers does not depend on the estimation for  $\boldsymbol{\tau}$  at previous step, the algorithm essentially searches in the space of  $\boldsymbol{\omega}$ . Hence, inserting a step size is only required for updating  $\boldsymbol{\omega}$  and we propose, following Bergsma (1997) to use the following basic updating equations with an added step size,  $0 < \text{step}^{(k)} \leq 1$ :

$$\boldsymbol{\omega}^{(k+1)} = \boldsymbol{\omega}^{(k)} + \text{step}^{(k)} \{ \mathbf{F}^{\omega\omega(k)} \mathbf{e}^{(k)} + \mathbf{F}^{\omega\tau(k)} h(\boldsymbol{\omega}^{(k)}) \},$$

where  $\mathbf{e}^{(k)} = \mathbf{n} - \hat{\boldsymbol{\mu}}^{(k)}$  and where  $\mathbf{F}^{\omega\omega(k)}$  and  $\mathbf{F}^{\omega\tau(k)}$  are two sections of  $\hat{\mathbf{F}}^{-1}$  at cycle  $k$ . We chose the step size by a simple step halving criterion, but more sophisticated step size rules could also be considered. A discussion on the choice of the step size may be found in Bergsma (1997). Note that the algorithm's updates take place in the rectangular space  $\mathbf{R}^t$  of  $\boldsymbol{\omega}$  rather than the not necessarily rectangular space  $\Lambda$  of the marginal log-linear parameters which may not be variation independent. The algorithm converges if it is started from suitable initial estimates of  $\boldsymbol{\omega}$  and  $\boldsymbol{\tau}$ . While usually a zero vector is a good choice for  $\boldsymbol{\tau}$ , we found empirically that the number of iterations to convergence can be reduced substantially by using as a starting value for  $\boldsymbol{\omega}$  an approximate maximum likelihood estimate based on results by Cox & Wermuth (1990) and Roddam (2004). At convergence, we obtain the maximum likelihood estimates  $\hat{\boldsymbol{\mu}} = \exp(\hat{\omega})$  and  $\hat{\boldsymbol{\pi}} = N^{-1} \hat{\boldsymbol{\mu}}$  and the asymptotic covariance matrices

$$\text{cov}(\hat{\omega}) = \hat{\mathbf{F}}^{\omega\omega}, \quad \text{cov}(\hat{\boldsymbol{\lambda}}) = \mathbf{H}_{sat} \hat{\mathbf{F}}^{\omega\omega} \mathbf{H}_{sat}^T, \text{ with } \mathbf{H}_{sat} = \mathbf{D}_{\hat{\boldsymbol{\mu}}} \mathbf{T}^T \mathbf{D}_{T\hat{\boldsymbol{\mu}}}^{-1} \mathbf{C}^T.$$

## 6. ANALYSIS OF SOME EXAMPLES

The examples of this section illustrate both the parameterizations and the fitting of marginal independence models. It is rare that a pure marginal independence model is useful in isolation and thus usually it is interpreted in combination with other graphical models. However, the problem of simultaneous testing of multiple marginal independencies in a general contingency table is often present in applications and it can be carried out



TABLE 5. *Parameters estimates of the 4-chain model for the data on symptoms of psychiatric patients under the multivariate logistic and the disconnected set parameterizations. The fit is  $\chi^2_5 = 8.61$ . Columns (1) and (2) are studentized estimates.*

Multivariate logistic param.			Disconnected set param.		
Margin	$\hat{\eta}$	(1)	Margin	Interaction	$\hat{\lambda}$ (2)
1	-0.28	-2.62	13	1	-0.28 -2.62
2	-0.13	-1.23		3	0.21 1.95
3	0.21	1.95		13	0.00
4	0.24	2.31	14	4	0.24 2.31
12	-0.72	-3.47		14	0.00
13	0.00		24	2	-0.13 -1.23
14	0.00			24	0.00
23	-1.12	-5.32	124	12	-0.72 -3.47
24	0.00			124	0.00
34	0.79	3.80	134	34	0.79 3.80
123	0.16	0.36		134	0.00
124	0.00		1234	23	-0.78 -1.80
134	0.00			123	0.14 0.20
234	-0.90	-2.03		234	-1.02 -1.63
1234	0.15	0.16		1234	0.15 0.16

with the technique discussed in this paper. All the computations were programmed in the R language (R Development Core Team, 2007).

**Example 9.** The 4-chain marginal independence model was fitted to the data on symptoms of psychiatric patients of Table 1 with the algorithm of Section 5. After 22 iterations, the algorithm leads to a chi-squared goodness of fit of 8.61 on 5 degrees of freedom. By comparison, the best graphical log-linear model has generators  $[12][234]$  with a deviance of 8.4 on 6 degrees of freedom. Thus, both models provide adequate interesting interpretations of the data. Table 5 summarizes the estimates of the 4-chain graph model, showing the parameter estimates and the studentized estimates under the multivariate logistic and the disconnected set parameterizations. In the multivariate logistic parameterization the two-factor parameters have the simple interpretation of marginal association coefficients. It must be kept in mind that they measure just the strength of marginal association between pairs of adjacent variables in the graph, but that the model includes higher order log-linear parameters which are not visible from the graph. For instance, both  $\hat{\eta}^{23} = -1.12$  and  $\hat{\eta}^{234} = -0.90$  are measures of association for variables  $X_2$  and  $X_3$ . In general, for any connected subgraph, all higher order log-linear parameters are expected. As explained in Section 4, the interpretation of the parameters necessarily depends on the chosen parameterization. For instance,  $\hat{\eta}^{23} = -1.12$  and  $\lambda_{23}^{1234} = -0.78$  are a marginal association measure and a conditional association measure respectively. The four-factor log-linear parameter is not significant, and a simpler reduced model with the additional

TABLE 6. *Data from U.S. General Social Survey.*

<i>S</i>	<i>C</i>	<i>G</i>	<i>A</i>	<i>J</i>	<i>F</i>			1			2			3		
					1	2	3	1	2	3	1	2	3	1	2	3
m	1	1	1		410	241	80	691	556	187	192	148	84			
				2	71	31	9	109	64	34	27	26	15			
			2	1	181	128	42	307	284	82	84	93	41			
				2	41	17	5	61	35	20	18	13	5			
	2	1	1		96	77	29	163	151	76	58	55	27			
				2	34	18	7	58	36	15	17	13	6			
		2	1		29	37	4	55	54	31	22	26	17			
				2	16	6	6	16	16	7	10	7	2			
		2	1		228	153	60	356	343	166	95	80	41			
				2	75	45	12	125	116	34	25	20	12			
f	1	1	1		552	353	145	899	793	265	180	162	94			
				2	98	60	15	186	122	47	40	23	14			
			2	1	133	74	33	219	164	66	36	47	24			
				2	25	15	1	54	40	13	14	6	4			
	2	1	1		228	153	60	356	343	166	95	80	41			
				2	75	45	12	125	116	34	25	20	12			
		2	1		41	25	13	64	56	22	15	14	11			
				2	17	6	1	19	18	6	3	3	2			

zero constraint on this parameter, has an adequate chi-squared goodness of fit of 8.63 on 6 degrees of freedom.

The following example concerns a larger contingency table including two ordinal variables with three levels. In the analysis these variables are treated as nominal variables using the baseline contrasts (2). Although the nature of the variables could be handled by using other more appropriate contrasts, as explained in Bartolucci *et al.* (2007), the fit of the marginal independence model is nevertheless invariant.

**Example 10.** Table 6 summarizes observations for 13067 individuals on 6 variables obtained from as many questions taken from the U.S. General Social Survey (Davis *et al.*, 2007) during the years 1972-2006. The variables are reported below with the original name in the GSS Codebook:

*C* CAPPUN: do you favor or oppose death penalty for persons convicted of murder? (1=favor, 2=oppose)

*F* CONFINAN: confidence in banks and financial institutions (1= a great deal, 2= only some, 3= hardly any)

*G* GUNLAW: would you favor or oppose a law which would require a person to obtain a police permit before he or she could buy a gun? (1=favor, 2=oppose)

*J* SATJOB: how satisfied are you with the work you do? (1 = very satisfied, 2= moderately satisfied, 3 = a little dissatisfied, 4= very dissatisfied). Categories 3 and 4 of SATJOB were merged together.

*S* SEX: Gender (f,m)

*A* ABRAPE: do you think it should be possible for a pregnant woman to obtain legal abortion if she became pregnant as a result of rape? (1= yes, 2 = no)

In data sets of this kind there are a large number of missing values and the table used in this example collects only individuals with complete observations. Therefore, the following exploratory analysis is intended to be only an illustration with a realistic example. From a first analysis of the data, the following marginal independencies are not rejected by the chi-squared goodness of fit test statistic

$$\begin{aligned} F \perp\!\!\!\perp CA \quad G \perp\!\!\!\perp JA \quad J \perp\!\!\!\perp GS \quad A \perp\!\!\!\perp FG \\ \chi_6^2 = 6.7 \quad \chi_5^2 = 3.3 \quad \chi_6^2 = 8.1 \quad \chi_5^2 = 2.1 \end{aligned}$$

and thus they suggest the independence model represented by the bi-directed graph in Figure 3(a). Fitting this model, under the multinomial sampling assumption, we obtain an adequate fit with a deviance of 17.29 on 17 degrees of freedom. The Aitchison and Silvey's algorithm converges after 13 iterations. The encoded independencies cannot be represented by a directed acyclic graph model with the same observed variables, because the graph contains at least one subgraph which is a chordless 4-chain. The disconnected set parameterization defined by the ordered decomposable sequence

$$\mathcal{M}_G = \{CF, FA, GJ, GA, JS, CFA, FGA, GJS, GJA, CFGJSA\}$$

is variation independent. Instead, by searching in the class of graphical log-linear models with the backward stepwise selection procedure of MIM (Edwards, 2000) we found a model with a deviance of 103.16 over 110 degrees of freedom. The model graph is shown in Figure 3(b). Other selection procedures show however that there are several equally well fitting models. The chosen undirected graph is slightly simpler (2 edge less) than the bi-directed graph. As anticipated, the number of constraints on parameters is however much higher. From the inspection of the studentized multivariate logistic estimates, we noticed that the higher order log-linear parameters are almost all not significant and thus we fitted a reduced model, by further restricting to zero all the log-linear parameters of order higher than two, obtaining a deviance of 108.34 on 118 degrees of freedom. The estimates of the remaining nonzero two-factor log-linear parameters are shown in Table 7. These are estimated local log odds-ratios in the selected two-way marginal tables and they have the expected signs. By comparison, the fitted non-graphical log-linear model with the graph of Figure 3(b), with additional zero constraints on the log-linear parameters of order higher than two, leads to a chi-squared goodness of fit of 118.49 on 119 degrees of freedom. Both models thus appear adequate.

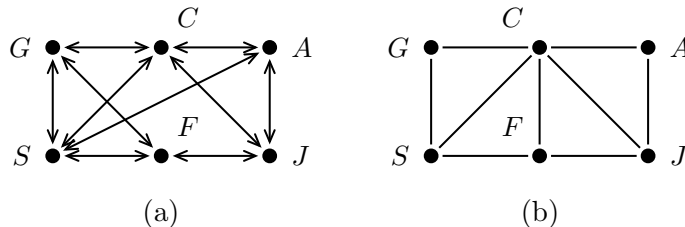


FIGURE 3. Data from the U.S. General Social Survey 1972-2006. (a) A bi-directed graph model ( $\chi_{17}^2 = 17.29$ ). (b) A graphical log-linear model ( $\chi_{110}^2 = 103.16$ ).

TABLE 7. *Estimates of two-factor log-linear parameters for the bi-directed graph model of Figure 3(a) with additional zero restrictions on higher order terms. The asterisks indicate the parameters for which the Wald statistic is significant.*

Margin	Parameter	Estimate	s.e.		Margin	Parameter	Estimate	s.e.	
$CG$	(1)	-0.38	0.048	*	$FG$	(1)	-0.01	0.047	
$CJ$	(1)	0.10	0.043	*		(2)	0.16	0.058	*
	(2)	0.14	0.058	*	$FJ$	(1)	0.29	0.044	*
$CS$	(1)	0.46	0.040	*		(2)	0.05	0.065	
$CA$	(1)	0.56	0.049	*		(3)	0.04	0.056	
$GS$	(1)	-0.77	0.042	*		(4)	0.36	0.072	*
$JA$	(1)	-0.21	0.051	*	$FS$	(1)	-0.004	0.040	
	(2)	-0.03	0.075			(2)	-0.35	0.051	*
$SA$	(1)	0.18	0.047	*					

The last example shows that sometimes the best fitted marginal independence model may be simpler than the best fitted directed acyclic model.

**Example 11.** The set of data in Table 8 is taken from the General Social Survey in Germany in 1998 (ALLBUS, 1998). In a selected population aged between 18 and 65, the answers of 1228 respondents are collected about the following 5 binary variables  $U$ , unconcerned about environment (yes, no);  $P$ , no own political impact expected (yes, no),  $E$ ; parents education, both at lower level (at most 10 years) (yes, no);  $A$ , age under 40 years (yes, no);  $S$ , gender (female, male). A possible ordering of the variables has been suggested by Wermuth (2003), who analyzed a superset of this data set and discussed a directed acyclic graph model. Using a similar ordering, limited to the variables here studied, we consider the variables  $\{A, S\}$  as purely explanatory,  $E$  and  $P$  as intermediate and  $U$  as final response. Our final well fitting directed acyclic graph model, shown in Figure 4(a), has a deviance 3.70 over 3 degrees of freedom. The subgraph for all the variables except gender  $S$  is complete. Specifically, the graph has an edge  $E \rightarrow U$ , indicating a direct effect of education on the final response. The model without the arrow  $E \rightarrow U$  has a worse goodness of fit  $\chi^2_{15} = 36.0$  and further it can be verified that the two-factor log-linear parameters  $EP$  and  $EA$  are large and significant. Model selection in the class of the graphical log-linear models does not lead to any sensible reduction whilst search in the class of bi-directed graph models shows that a special structure of marginal independencies holds.

TABLE 8. *Data from the German General Social Survey in 1998.*

		$U$ yes				no				
		$S$ f		m		f		m		
$A$	$E$	$P$	yes	no	yes	no	yes	no	yes	no
no	yes		6	8	7	27	66	186	24	230
	no		4	0	1	9	8	64	4	60
yes	yes		2	2	11	6	28	159	16	130
	no		0	1	0	2	4	75	8	80

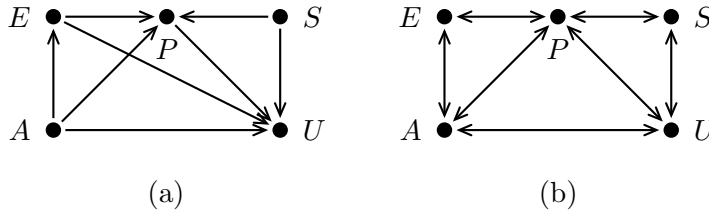


FIGURE 4. Two graphical models fitted to data from the General Social Survey in Germany, 1998. (a) A directed acyclic graph model:  $\chi^2_3 = 3.70$ . (b) A bi-directed graph model:  $\chi^2_5 = 5.91$ .

The final selected bi-directed graph, represented in Figure 4(b), represents the marginal independencies  $S \perp\!\!\!\perp A, E$  and  $E \perp\!\!\!\perp S, U$ . The bi-directed graph contains the chordless 4-chain  $EAUS$  and thus it is not Markov equivalent to any directed acyclic graph in the five variables. This suggests that the directed acyclic graph model conceals some distortions due to the presence of latent variables. Also in this case, the disconnected set parameterization defined by the sequence  $\mathcal{M}_G = (GE, GF, AE, GFE, GEA, ABEFG)$  leads to a variation independent parameterization because it can be verified that the sequence  $\mathcal{M}_G$  is order decomposable.

## 7. DISCUSSION

The discrete models based on marginal log-linear models by Bergsma & Rudas (2002) form a large class that includes several discrete graphical models. The undirected graph models and the chain graph models under the classical (Lauritzen, Wermuth, Frydenberg) interpretation can be parameterized as marginal log-linear models. For an introduction see Rudas *et al.* (2006). This paper shows that the discrete bi-directed graph models under the global Markov property are included in the same class by specifying the constraints appropriately. In general, three main criteria were considered in choosing a marginal log-linear parameterization.

- (a) Upward compatibility: if the parameters have a meaning that is invariant across different marginal distributions, then the interpretations remain the same when a sub-model is chosen. We saw that the multivariate logistic parameterization has this property.
- (b) Modelling considerations: the parameterization should contain all the parameters that are of interest for the problem at hand. For example, in a regression context where some variables are prior to others, effect parameters conditional on the explanatory variables are most meaningful. In the seemingly unrelated regression problem of Example 7, the chosen parameters have the interpretation of logistic regression coefficients.
- (c) Variation independence: if the parameter space is the whole Euclidean space, this has certain advantages. First, the interpretations are simpler, because in a certain sense different parameters measure different things. Second, in a Bayesian context, prior specification is easier. Finally, the problem of out-of-bound estimates when transforming the parameters to probabilities is avoided. In the examples, we always

found a variation independent parameterization, but a characterization of the class of bi-directed graphs admitting a variation independent complete and hierarchical marginal log-linear parameterization is an open problem.

The three criteria are in some cases conflicting: typically variation independence is obtained at the expense of upward compatibility.

The multivariate logistic parameterization has a purpose similar to that of the Möbius parameterization recently proposed by Drton & Richardson (2007) for binary marginal independence models, which is based on a minimal set of marginal probabilities identifying the joint distribution. These authors discuss the type of constraints on the Möbius parameters needed to specify a marginal independence, showing that they take a simple multiplicative form. The same constraints are defined by zero restrictions on marginal log-linear parameters in our approach. Even if the parametric space can be awkward, this problem is handled by a fitting algorithm that operates in the space of the expected frequencies, while the parameters are used only to define the independence constraints. Moreover, the definition of the models through the complete specification of the marginal log-linear parameters gives some advantage when there is a mixture of nominal and ordinal variables because it allows to define appropriate parameters for both types of variables using the theory of generalized marginal interactions by (Bartolucci *et al.*, 2007). This opens the way to defining subclasses of discrete graphical models specifying equality and inequality constraints.

The proposed algorithm for maximum likelihood fitting of the bi-directed graph model is a very general algorithm of constrained optimization based on Lagrange multipliers. It is essentially based on Aitchison & Silvey (1958) as later developed by Bergsma (1997). Similar algorithms have been proposed, for instance, by Molenberghs & Lesaffre (1994), Glonek & McCullagh (1995), Lang (1996) and further generalized by Colombi & Forcina (2001). Its main advantage is its generality (it can be applied to all models defined by constraints on the marginal log-linear parameters). As previously stated, the algorithm does not require further iterative procedures for computing, at each step, the inverse transformation from the marginal log-linear parameters to the cell probabilities. Thus, the risk of not compatible estimates that could arise for the lack of variation independence is avoided. The disadvantage is that, as for many gradient-based algorithms of this type, convergence is not guaranteed and that it requires the computation of a large expected information matrix. However, empirically, convergence is achieved in a relative few number of iterations by including a step adjustment. An alternative algorithm with convergence guarantees is the Iterated Conditional Fitting algorithm, proposed by Drton & Richardson (2007) for binary bi-directed graph models in the Möbius parameterization. A comparison between the two algorithms in terms of performance, speed and memory requirements needs further investigation.

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